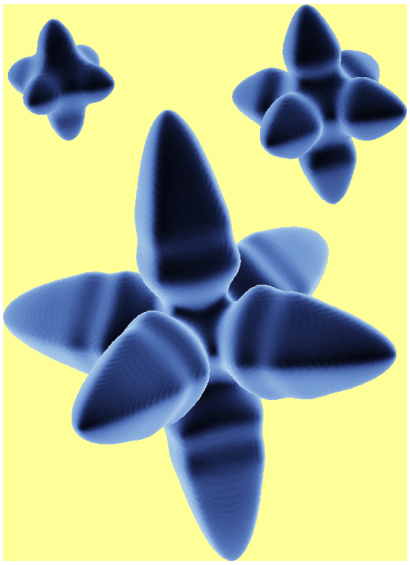
VI.H Simulations of Three-Dimensional Solidification: Dendritic Structures

Introduction: Dendritic (snow-flake like) growth is a complex pattern formation process that takes place during the solidification of engineering materials ranging from Al-based alloys for the automotive industry to Ni-based superalloys for the aircraft industry. The growth morphology of dendrites determines the microstructure of these materials. Thus, the ability to accurately model this growth is of fundamental importance for predicting essential mechanical properties controlled by the microstructure, such as strength and durability. Yet, the prediction of the microstructure remains often qualitative and unreliable in a variety of industrial processes (including welding, casting, sintering, etc.). There are two major obstacles. First, microstructures form via the motion of anisotropic interfaces (solid-liquid, solid-solid, and grain boundaries). Thus, one is faced with the difficulty of tracking the time evolution of two-dimensional surfaces of arbitrary complex shapes. Second, fast atomic scale processes determine the thermodynamic and kinetic properties, which in turn govern the response of an interface to a driving force (diffusion flux, stress, etc.). However, the macroscopic length and time scales on which the microstructure evolves are several orders of magnitude larger than the atomic scales. Reliably bridging the gap between these microscopic and macroscopic scales has remained a computational challenge.

Results: A major advance in coping with both difficulties has occurred recently in solidification modeling. The figure illustrates the first fully quantitative simulation of the growth of a three-dimensional dendrite, which is the fundamental building block of alloy microstructures. In this example, bridging the micro-macro gap has involved treating scales ranging from a nanometer capillary length to a millimeter diffusion length. It was found that a weak anisotropy in surface energy has a profound influence on the growth morphology of dendrites and thus the properties of cast products.



Three snapshots of dendritic growth

Calculational Notes: These calculations were made possible by developing a computationally efficient phase-field model that allows tracking an arbitrarily complex interface shape in three dimensions. The work required massively parallel implementation on the Cray T3E at NERSC. Three snapshots of the solid-liquid interface are shown following the morphological instability of a spherical nucleus. One second of real time corresponds to 100 hours of CPU time using 64 processors of the Cray T3E.

Significance: This work represents one of the earliest successful efforts to bridge the micro-macro gap. The surface energy anisotropy is an input parameter of the model that presently needs to be determined experimentally, which is not yet feasible in metallic systems. Therefore, atomic scale first principles calculations must predict the required critical parameter (the surface energy anisotropy) independent of experiment. The computing power available with SSI should also permit extension of this work to incorporate the convection (fluid motion) that is universally present in castings and strongly influences the microstructure. Thus, we are on the verge of realistically modeling one of the most technically important and most basic of materials processing phenomena.